REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

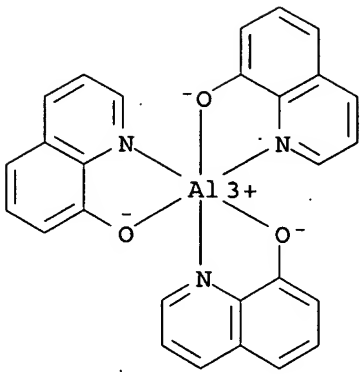
(FILE 'HOME' ENTERED AT 09:09:57 ON 15 NOV 2005)

FILE 'REGISTRY' ENTERED AT 09:10:16 ON 15 NOV 2005
L1 STRUCTURE UPLOADED
L2 18 S L1
E ALQ3/CN
L3 1 S E3

FILE 'CAPLUS' ENTERED AT 09:13:07 ON 15 NOV 2005
L4 4979 S L3
L5 124 S FACIAL ISOMER?
L6 14 S L4 AND L5

=> d l3
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 2085-33-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Aluminum, tris(8-quinolinolato)- (6CI, 7CI, 8CI)
CN Aluminum, tris(8-quinolinolato-N1,O8)-
OTHER NAMES:
CN 8-Hydroxyquinoline aluminum
CN Al 8Q
CN **Alq3**
CN Aluminum 8-hydroxyquinolinate
CN Aluminum oxinate
CN Aluminum tris(8-hydroxyquinolinate)
CN Aluminum tris(8-quinolinolate)
CN Aluminum, tris(8-hydroxyquinolinato)-
CN Hydroxyquinoline aluminum
CN Tri-8-quinolinolatoaluminum
CN Tris(8-hydroxyquinolato)aluminum
CN Tris(8-hydroxyquinolinate)aluminum
CN Tris(8-hydroxyquinolinato)aluminum
CN Tris(8-hydroxyquinolinol-N1,O8)aluminum
CN Tris(8-quinolinol)aluminum
CN Tris(8-quinolinolato)aluminum
CN Tris(8-quinolinolato)aluminum(III)
CN Tris-(8-hydroxyquinoline)aluminum
DR 11094-99-8, 24731-66-6
MF C27 H18 Al N3 O3
CI CCS, COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMLIST, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, MRCK*, PIRA, RTECS*, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4958 REFERENCES IN FILE CA (1907 TO DATE)
22 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
4979 REFERENCES IN FILE CAPLUS (1907 TO DATE)
44 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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STN- Structure Search 11/15/05

10/517,203

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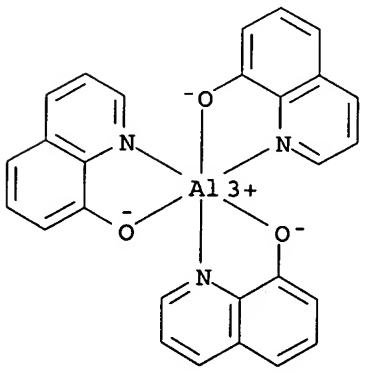
L6 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:599421 CAPLUS
DOCUMENT NUMBER: 143:255825
TITLE: Relationships between light-emitting properties and different isomers in polymorphs of tris(8-hydroxyquinoline) aluminum(III) (Alq3) analyzed by solid-state 27Al NMR and density functional theory (DFT) calculations
AUTHOR(S): Kaji, Hironori; Kusaka, Yasunari; Onoyama, Goro; Horii, Fumitaka
CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan
SOURCE: Japanese Journal of Applied Physics, Part 1: Regular Papers, Brief Communications & Review Papers (2005), 44(6A), 3706-3711
CODEN: JAPNDE
PUBLISHER: Japan Society of Applied Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structures of tris(8-hydroxyquinoline) Al(III) (Alq3) in the different polymorphs, α-, γ-, and δ-Alq3, and in the amorphous state, amo-Alq3, were analyzed by solid-state 27Al NMR. The local structures of α- and amo-Alq3 are similar; both samples are composed of the meridional isomer and are locally disordered. No evidence of the existence of the **facial isomer** is found even for amo-Alq3. But the isomeric states of γ- and δ-Alq3 are facial. The 27Al NMR spectrum of δ-Alq3 is influenced by intermol. interactions, whereas that of γ-Alq3 is determined only by a single facial Alq3 mol., suggesting that intermol. interactions are negligible for γ-Alq3. This result is closely related to the exptl. observed good solubility of γ-Alq3. D. functional theory (DFT) calcns. support the identification of the isomeric state and the effect of the intermol. interactions. A clear correlation between the isomeric state and the fluorescence wavelength is found, indicating that the isomeric state of Alq3 is a crucial factor for the light-emitting properties.

IT **2085-33-8**, Al 8q
RL: PRP (Properties)
(relationships between light-emitting properties and different isomers in polymorphs of tris(8-hydroxyquinoline) aluminum(III) (Alq3) analyzed by solid-state 27Al NMR and d. functional theory (DFT) calcns.)

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



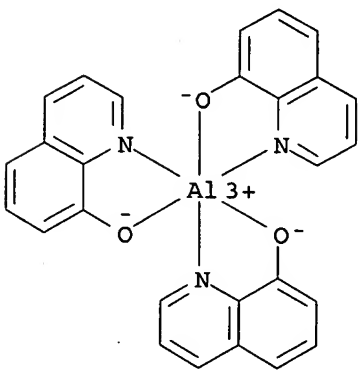
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1064091 CAPLUS
DOCUMENT NUMBER: 143:201886
TITLE: Delayed fluorescence and phosphorescence of tris-(8-hydroxyquinoline)aluminum (Alq3) and their temperature dependence
AUTHOR(S): Coelle, M.; Gaerditz, C.
CORPORATE SOURCE: Experimentalphysik II and Bayreuther Institut fuer Makromolekuelforschung (BIMF), Universitaet Bayreuth, Bayreuth, D-95440, Germany
SOURCE: Journal of Luminescence (2004), 110(4), 200-206
CODEN: JLUMA8; ISSN: 0022-2313
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper reports on delayed luminescence measurements of tris(8-hydroxyquinoline)aluminum (Alq3) after optical excitation; these identify 2 bands in the emission spectrum: delayed fluorescence and phosphorescence. This is shown for different crystalline phases and for evaporated films. The assignment of the low-energy band to the phosphorescence is confirmed by lifetime measurements, and triplet energies of the meridional isomer in the α-phase and the **facial isomer** in the δ-phase are determined from the well-resolved vibronic progressions of the phosphorescence as 2.11 ± 0.1 and 2.16 ± 0.1 eV, resp. Lifetimes of the delayed fluorescence and the phosphorescence are determined for a temperature range from 6 to 150 K, and the temperature dependence of the delayed luminescence were measured.

IT **2085-33-8**, Tris(8-hydroxyquinolinato)aluminum
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(delayed fluorescence and phosphorescence and their temperature dependence of)
RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

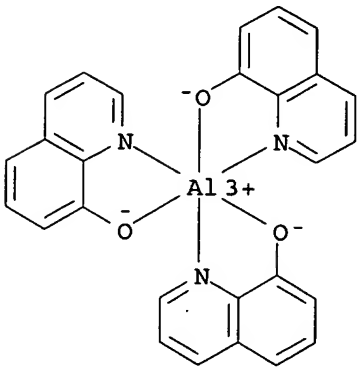
L6 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1026829 CAPLUS
DOCUMENT NUMBER: 142:164738
TITLE: The triplet state in tris-(8-hydroxyquinoline)aluminum

AUTHOR(S): Colle, M.; Garditz, C.; Braun, M.
CORPORATE SOURCE: Experimentalphysik II and Bayreuther Institut fuer Makromolekuelforschung, Universitaet Bayreuth, Bayreuth, D-95440, Germany
SOURCE: Journal of Applied Physics (2004), 96(11), 6133-6141
CODEN: JAPIAU; ISSN: 0021-8979
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This paper presents the characterization of the triplet state in tris-(8-hydroxyquinoline)aluminum (Alq3). An emission spectrum of Alq3, namely, the phosphorescence, is presented for crystalline and amorphous Alq3, which enables direct study of the T1 S0 transition. The assignment of this spectrum to the phosphorescence is further confirmed by temperature-dependent measurements and comparison with the delayed fluorescence.

The triplet energies of the meridional and **facial isomer** (in α- and δ-Alq3) are determined from the well-resolved vibronic progressions of the phosphorescence as 2.11 ± 0.1 and 2.16 ± 0.1 eV, resp. Also, the lifetime of the triplet state is measured for a temperature range from 6 to 150 K. These temperature-dependent measurements also identify a

so far unknown phase transition of Alq3 at .apprx.50 K. Optically detected magnetic resonance at a zero field is used to measure the characteristic zero-field splitting parameters (|E|=0.0114 cm-1 and |D|=0.0630 cm-1), and these are discussed in terms of a mol. symmetry and contribution of different ligands and suggest a mini-exciton-like behavior of the triplet state on the 3 ligands of the Alq3 mol. All these measurements are performed on different crystalline phases (α- and δ-Alq3) and on evaporated amorphous films. The differences observed for the δ-phase are consistent with the reduced intersystem crossing and thus with the **facial isomer** in this phase.

IT **2085-33-8**, Tris-(8-hydroxyquinoline)aluminum
RL: PRP (Properties)
(triplet state in (8-hydroxyquinoline)aluminum film)
RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:944547 CAPLUS
DOCUMENT NUMBER: 142:122163
TITLE: Study of the interaction of tris-(8-hydroxyquinoline) aluminum (Alq3) with potassium using vibrational

spectroscopy: Examination of possible isomerization upon K doping

AUTHOR(S): Sakurai, Y.; Hosoi, Y.; Ishii, H.; Ouchi, Y.; Salvan, G.; Kobitski, A.; Kampen, T. U.; Zahn, D. R. T.; Seki, K.

CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Nagoya University, Nagoya, 464-8602, Japan

SOURCE: Journal of Applied Physics (2004), 96(10), 5534-5542
CODEN: JAPIAU; ISSN: 0021-8979

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

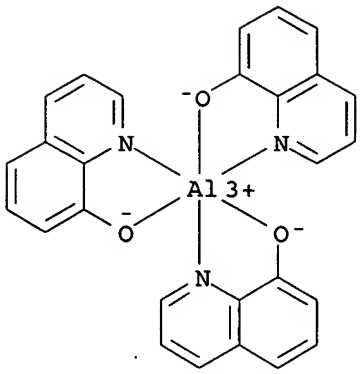
LANGUAGE: English

AB The geometrical structure of K-doped Alq3 [tris-(8-hydroxyquinoline) Al] and the interaction between the Alq3 mol. and K were studied using IR reflection absorption spectroscopy (IRRAS), surface-enhanced Raman scattering (SERS), and d. functional theory calcns. A major aim of this study was to examine the theor. predicted isomerization of Alq3 mols. from the meridional form to the facial form upon alkali-metal doping. The observed spectra show significant changes with the deposition of K on a thin Alq3 film. The calculated IR spectra of the K-Alq3 complex differ significantly between the meridional and facial forms, and the calcn. for the meridional form agrees fairly well with the observed spectrum. This demonstrates that (1) the Alq3 mol. does not change to a **facial isomer** with the deposition of K, but retains the meridional form, in contrast to the reported theor. prediction, and (2) the structure of the complex as evaluated from geometry optimization is reliable. Also the calculated IR spectrum of the K-Alq3 complex with Alq3 in its meridional form is significantly different from that of the isolated anion in the same isomeric form, which probably reflects nonuniform interaction between K and the 3 ligands of Alq3. However, the calculated spectra of Alq3 and the K-Alq3 complex in the facial form are similar, possibly because the K atom in the suggested structure lies on the axis of 3-fold symmetry, leading to an equivalent effect on the 3 ligands. Even though vibrational spectra of alkali-metal-doped organic materials are usually interpreted from an isolated anion, care should be taken in interpreting the spectra of doped organic materials without considering the presence of the counterion. The observed SERS spectra and theor. calcns. of the Raman spectra show similar trends when compared to the IRRAS results. Vibrational spectroscopy can be used as a sensitive tool for discerning subtle differences between isomers as well as between complexes and isolated anions.

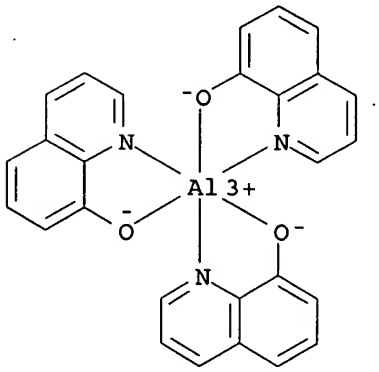
IT **2085-33-8DP**, Alq3, potassium complex
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); PYP (Physical process); PREP (Preparation); PROC (Process)
(K-doped Alq3; vibrational spectra of Alq3-K interaction upon K doping with possible isomerization)

RN 2085-33-8 CAPLUS

CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



IT **2085-33-8**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(K-doped Alq3; vibrational spectra of Alq3-K interaction upon K doping with possible isomerization)
RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

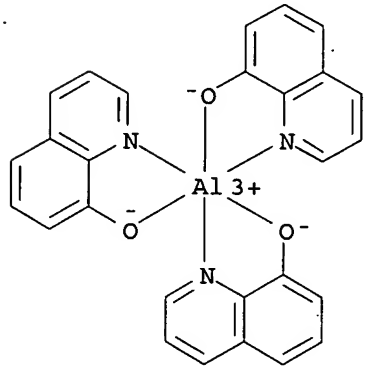
L6 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:469047 CAPLUS
DOCUMENT NUMBER: 142:64193
TITLE: Thermal, structural and photophysical properties of the organic semiconductor Alq3
AUTHOR(S): Coelle, M.; Bruetting, W.
CORPORATE SOURCE: Experimentalphysik II and Bayreuther Institut fuer Makromolekuelforschung (BIMF), Universitaet Bayreuth, Bayreuth, 95440, Germany
SOURCE: Physica Status Solidi A: Applied Research (2004), 201(6), 1095-1115
CODEN: PSSABA; ISSN: 0031-8965
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. This review describes the thermal, structural and photophys. properties of different polycryst. phases of the organic semiconductor Alq3. In particular the new blue luminescent δ-phase is shown to contain the **facial isomer.** The results obtained by using

differential scanning calorimetry, X-ray diffraction, IR spectroscopy, transient and delayed photoluminescence measurements clearly demonstrate the existence of this isomer. From the results presented it is now possible to obtain the pure **facial isomer** of Alq3 in large quantities, providing the basis for further investigations to determine its effects on the performance of organic light-emitting diodes. Furthermore, recent results on the properties of the triplet states in Alq are presented. This includes the population of the electronic excited triplet state due to inter-system crossing and the spectrum of the phosphorescence.

IT **2085-33-8**, Alq3
RL: PRP (Properties)
(thermal, structural and photophys. properties of the organic semiconductor Alq3)

RN 2085-33-8 CAPLUS

CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:880346 CAPLUS

DOCUMENT NUMBER: 140:86312

TITLE: Characterization of isomers in aluminum tris(quinoline-8-olate) by one-dimensional 27Al nuclear magnetic resonance under magic-angle spinning

AUTHOR(S): Utz, Marcel; Nandagopal, Magesh; Mathai, Mathew; Papadimitrakopoulos, Fotios

CORPORATE SOURCE: Institute of Materials Science and Department of Physics, University of Connecticut, Storrs, CT, 06269, USA

SOURCE: Applied Physics Letters (2003), 83(19), 4023-4025
CODEN: APPLAB; ISSN: 0003-6951

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

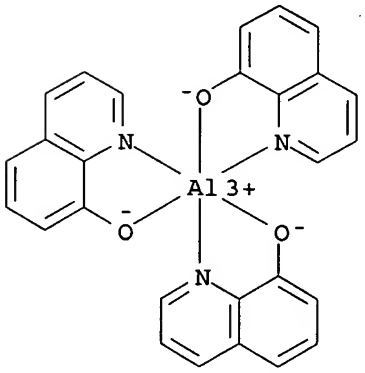
AB Solid-state 27Al NMR spectra under magic-angle spinning of different forms of aluminum tris(quinoline-8-olate) (Alq3) are presented. Alq3 is an organometallic complex of great importance in the context of organic light-emitting diodes. The authors' results demonstrate a strong difference in the asymmetry of the elec. field gradient (EFG) tensor at the aluminum site between the α and the recently discovered δ polymorph of Alq3. While the EFG is nearly planar ($\eta \approx 1$) in the α phase, it is nearly axially sym. ($\eta \approx 0$) for the δ phase. This result provides strong support to the hypothesis that the δ phase contains the **facial isomer** of Alq3.

While the spectra of both the α and the δ polymorphs exhibit sharp features, highly disordered forms of Alq3 obtained from rapid vapor deposition onto a cold substrate, yield broadened spectra, indicating substantial structural disorder in the local geometry of different Alq3 mols.

IT **2085-33-8**
RL: PRP (Properties)
(27Al MAS NMR characterization of isomers in aluminum tris(quinoline-8-olate))

RN 2085-33-8 CAPLUS

CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:756517 CAPLUS

DOCUMENT NUMBER: 140:11871

TITLE: Characterization of isomers in solid aluminum tris-(quinoline-8-olate) by NMR

AUTHOR(S): Nandagopal, Magesh; Mathai, Mathew; Papadimitrakopoulos, Fotios; Utz, Marcel

CORPORATE SOURCE: Institute of Materials Science, University of Connecticut, Storrs, CT, 06269, USA

SOURCE: Materials Research Society Symposium Proceedings (2003), 771(Organic and Polymeric Materials and Devices), 267-272
CODEN: MRSPDH; ISSN: 0272-9172

PUBLISHER: Materials Research Society

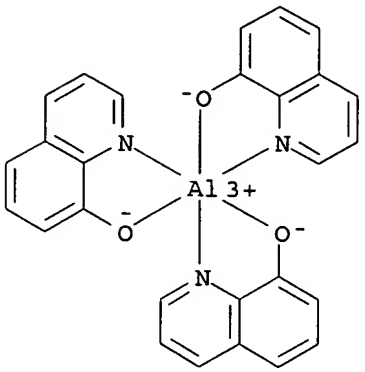
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Al tris-(quinoline-8-olate) (Alq3) is the most widely used electron transport material for organic light emitting diodes. The Alq3 mol. exists as two different isomers: meridianal and facial, which differ by the symmetry of the arrangement of ligands around the Al ion. Various crystalline polymorphs of Alq3 were identified to contain one of these isomers. The authors present exptl. results that show that the facial and meridianal isomers of Alq3 can be distinguished in the solid state by 27Al NMR spectroscopy under magic angle spinning (MAS). The authors' results prove that the recently discovered δ-phase of Alq3 exclusively contains the **facial isomer.** The same technique is also used to characterize the amorphous deposit of Alq3 showing that it is the meridianal isomer that predominantly exists in the amorphous state.

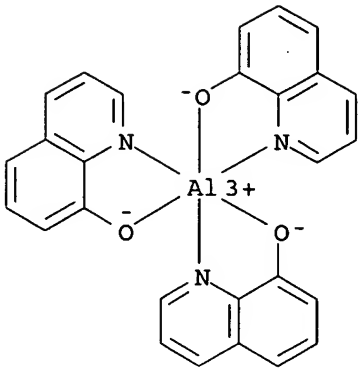
IT **2085-33-8**, Aluminum tris(8-hydroxyquinolinato)
RL: PRP (Properties)
(characterization of isomers in solid aluminum tris-(quinoline-8-olate)

by 27Al NMR)
RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:756477 CAPLUS
DOCUMENT NUMBER: 140:10314
TITLE: Energetics of mer/fac isomers in metal tris(8-hydroxyquinoline) chelates: Implications on charge conduction in organic light-emitting devices
AUTHOR(S): Ferris, Kim F.; Sapochak, Linda S.; Rodovsky, Deanna; Burrows, Paul E.
CORPORATE SOURCE: Materials Science Division, Pacific Northwest National Laboratory, Richland, WA, 99352, USA
SOURCE: Materials Research Society Symposium Proceedings (2003), 771(Organic and Polymeric Materials and Devices), 17-22
CODEN: MRSPDH; ISSN: 0272-9172
PUBLISHER: Materials Research Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electronic structure calcns. for the mer and fac-isomers of aluminum tris(8-hydroxyquinoline) (Alq3) and the methyl-substituted series, nMeq3Al (n = 3-7) are presented. From these data, we estimate their relative abundances in Alq3 thin films and the resultant trap state energies. Ab initio computations performed at the SCF level suggest a significantly higher stability (6-7.5 kcal/mol) of the mer isomer over the facial form, whereas MP2 treatment of electron correlation effects lowers the difference to 4-4.5 kcal/mol. Substitution of the Al3+ metal ion with the larger ions Ga3+ and In3+ increases the energetic preference of the meridional form by 2.7 kcal/mol and decreases it by 0.8 kcal/mol, resp. Trap state energies calculated by previously proposed methodologies show little difference between mer and fac trap states. These results suggest that the existence of the **facial isomer** in thin films of metal tris-quinolates is unlikely to significantly affect charge conduction.
IT **2085-33-8**
RL: PRP (Properties)
(energetics of mer/fac isomers in metal tris(8-hydroxyquinoline) chelates with implications for charge conduction in LEDs)
RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



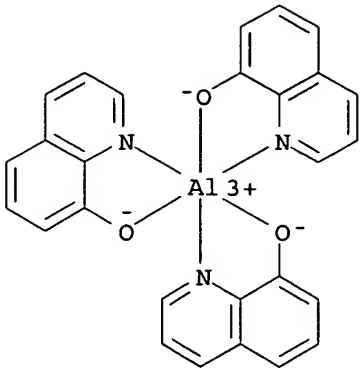
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:501462 CAPLUS
DOCUMENT NUMBER: 139:313794
TITLE: Vibrational analysis of different crystalline phases of the organic electroluminescent material aluminium tris(quinoline-8-olate) (Alq3)
AUTHOR(S): Coelle, Michael; Forero-Lenger, Stefan; Gmeiner, Juergen; Bruetting, Wolfgang
CORPORATE SOURCE: University of Bayreuth, Experimental Physics II, Bayreuth, 95440, Germany
SOURCE: Physical Chemistry Chemical Physics (2003), 5(14), 2958-2963
CODEN: PPCPFQ; ISSN: 1463-9076
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The isomerism of the Alq3 mol. was investigated by applying IR spectroscopy to two different crystalline phases of aluminum tris(quinoline-8-olate) (α-Alq3 and δ-Alq3). Significant differences between the two phases were found in the IR spectra, which can be explained in terms of the different symmetries of the facial and meridional isomer. Addnl., intermol. interactions of the Alq3 mols. due to crystallinity were taken into account. The results suggest that α-Alq3 consists of the meridional isomer, while the recently discovered blue luminescent δ-phase is composed of the **facial isomer** of the Alq3 mol.

IT **2085-33-8**
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(vibrational anal. of different crystalline phases of organic electroluminescent material aluminum tris(quinoline-8-olate))

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



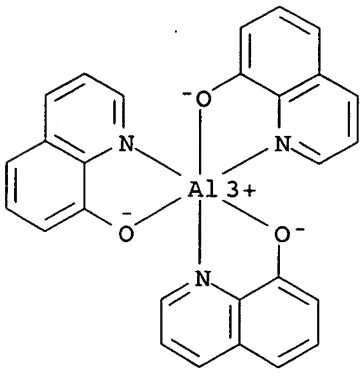
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:215463 CAPLUS
DOCUMENT NUMBER: 138:359647
TITLE: Luminescent Compounds fac- and mer-Aluminum Tris(quinolin-8-olate). A Pure and Hybrid Density Functional Theory and Time-Dependent Density Functional Theory Investigation of Their Electronic and Spectroscopic Properties
AUTHOR(S): Amati, Mario; Lelj, Francesco
CORPORATE SOURCE: La.MI Dipartimento di Chimica and LaSCAMM INSTM Sezione Basilicata, Universita della Basilicata, Potenza, 85100, Italy
SOURCE: Journal of Physical Chemistry A (2003), 107(14), 2560-2569
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB D. functional theory and time-dependent d. functional theory have been applied to describe the ground and excited states and the spectral characteristics of the meridianal and **facial isomers** of aluminum tris(quinolin-8-olate) (Alq3). Vertical absorption wavelengths and oscillator strengths of both meridianal Alq3 and facial Alq3 have been computed up to about 255 nm (4.86 eV) and compared with exptl. data. Exptl. meridianal Alq3 absorption band locations are well reproduced by the computations, allowing easy assignment of the absorption bands. The facial Alq3 absorption spectrum has been computed, and a detailed comparison of the excited state characteristics of the two isomers has been addressed for pointing out differences in absorption and emission properties. This work suggests that the facial Alq3 may be the constituent of the recently reported Alq3 crystalline phase known as the δ-phase. This is an important new material for understanding the Alq3 solid-state properties and for a possible organic light-emitting diode fabrication. Some suggestions to exptl. distinguish the two isomers have been presented. Furthermore, information about the excited-state kinetics of both the isomers and properties of their emissive excited states has been gained. Both the hybrid B3LYP and the pure BLYP, LSDA, BPW91, and LB94 exchange-correlation functionals have been tested, and the B3LYP functional clearly seems to be the best choice for this class of mols.

IT **2085-33-8**
RL: PRP (Properties)
(pure and hybrid d. functional theory and time-dependent d. functional theory investigation of luminescent fac- and mer-Alq3 isomers and their electronic and spectroscopic properties)

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



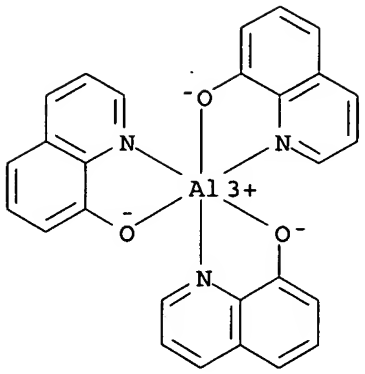
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:884523 CAPLUS
DOCUMENT NUMBER: 138:212161
TITLE: The structure of the blue luminescent δ-phase of tris(8-hydroxyquinoline)aluminum(III) (Alq3)
AUTHOR(S): Coelle, Michael; Dinnebier, Robert E.; Bruetting, Wolfgang
CORPORATE SOURCE: Universitaet Bayreuth, Experimentalphysik II, Bayreuth, 95440, Germany
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2002), (23), 2908-2909
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The existence of the **facial isomer** in the δ-phase of Alq3 is proven by x-ray structural anal., revealing that both the different mol. structure and the weaker overlap of the π-orbitals of hydroxyquinoline ligands belonging to neighboring Alq3 mols. as compared to other phases (α, β) probably are the origin of the significantly different optical properties of δ-Alq3.

IT **2085-33-8**, Aluminum tris(8-hydroxyquinolinato)
RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(structure of blue luminescent δ-phase of tris(8-hydroxyquinoline)aluminum(III))

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



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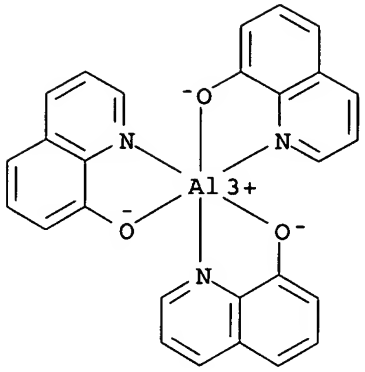
L6 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:443523 CAPLUS
DOCUMENT NUMBER: 137:192158
TITLE: Are UV-Vis and luminescence spectra of Alq3 [aluminum tris(8-hydroxy quinolinate)] δ-phase compatible with the presence of the fac-Alq3 isomer? A TD-DFT investigation
AUTHOR(S): Amati, M.; Lelj, F.
CORPORATE SOURCE: INSTM Sezione Basilicata, Dipartimento di Chimica and LASCAMM, LaMI, Universita' della Basilicata, Potenza, I-85100, Italy
SOURCE: Chemical Physics Letters (2002), 358(1,2), 144-150
CODEN: CHPLBC; ISSN: 0009-2614
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Recently a new crystalline phase of Al tris(8-hydroxyquinolinate) (Alq3) called δ-phase is reported. From luminescence data, the presence of the **facial isomer** was suggested. Using time dependent d. functional theory calcns. the authors compared the spectral features of meridianal and facial Alq3. Comparisons between the two isomers were used to confirm the presence of facial Alq3 in δ-phase crystals. The interpretation of some characteristics of the more studied meridianal isomer was suggested.

IT **2085-33-8**, Aluminum tris(8-hydroxy quinolinato)
RL: PRP (Properties)
(TD-DFT investigation of UV-Vis and luminescence spectra of Alq3 [aluminum tris(8-hydroxy quinolinate)] δ-phase and presence of fac-Alq3 isomer)

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



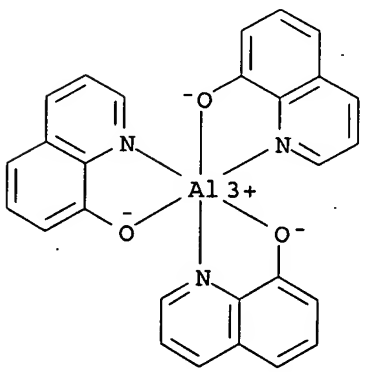
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:751660 CAPLUS
DOCUMENT NUMBER: 136:46087
TITLE: Nondispersive electron transport in Alq3
AUTHOR(S): Malliaras, George G.; Shen, Yulong; Dunlap, David H.; Murata, Hideyuki; Kafafi, Zakya H.
CORPORATE SOURCE: Department of Materials Science and Engineering, Cornell University, Ithaca, NY, 14853, USA
SOURCE: Applied Physics Letters (2001), 79(16), 2582-2584
CODEN: APPLAB; ISSN: 0003-6951
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors have studied room temperature electron transport in amorphous films of tris(8-hydroxyquinolinolato)aluminum (Alq3) with the time-of-flight technique. Nondispersive photocurrent transients indicate the absence of intrinsic traps in well-purified films. Exposure of the films to an ambient atmospheric results in highly dispersive transport, indicating that oxygen is a likely candidate for a trapping site. The mobility was found to obey the Poole-Frenkel law. The authors use the correlated disorder model to determine an effective dipole moment for Alq3, and the corresponding meridional to **facial isomeric** ratio.

IT **2085-33-8**
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(nondispersive electron transport in Alq3)

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:391231 CAPLUS
DOCUMENT NUMBER: 135:186995
TITLE: A new crystalline phase of the electroluminescent material tris(8-hydroxyquinoline) aluminum exhibiting blueshifted fluorescence
AUTHOR(S): Braun, M.; Gmeiner, J.; Tzolov, M.; Coelle, M.; Meyer, F. D.; Milius, W.; Hillebrecht, H.; Wendland, O.; von Schutz, J. U.; Brutting, W.
CORPORATE SOURCE: 3. Institute of Physics, University of Stuttgart, Stuttgart, 70550, Germany
SOURCE: Journal of Chemical Physics (2001), 114(21), 9625-9632
CODEN: JCPSA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors report on two different crystalline phases of tris(8-hydroxyquinoline) Al (Alq3) which were obtained by thermal sublimation in a horizontal glass tube. These phases were studied by x-ray powder diffraction, Raman and IR spectroscopy, and low temperature photoluminescence measurements. Apart from the already known α phase the authors could identify a new crystalline phase of Alq3 (δ-Alq3) showing blueshifted fluorescence. As compared to the α phase this new phase was characterized by a larger unit cell volume, a reduced number of Raman lines in the energy range between 70 and 700 cm-1, a blueshift of the photoluminescence maximum by .apprx.0.2 eV, and a decreased intersystem crossing to the triplet state. These differences are interpreted in terms of the isomers of the Alq3 mol. Probably the new phase contains the **facial isomer**, whereas in the other phases only the meridianal isomer is reported. Low temperature photoluminescence spectra show a well-resolved vibronic progression with about the same spacing of 550 cm-1 for both crystalline phases of Alq3. Site-selective photoluminescence measurements reveal the existence of an addnl. red shifted featureless emission, which is ascribed to energy relaxation into low-lying states.

IT **2085-33-8**, Aluminum tris(8-hydroxyquinolinato)
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(a new crystalline phase of electroluminescent material tris(8-hydroxyquinoline) aluminum exhibiting blueshifted fluorescence)

RN 2085-33-8 CAPLUS
CN Aluminum, tris(8-quinolinolato-κN1,κO8)- (9CI) (CA INDEX NAME)